

Computer simulation of field ion images of nanoporous structure in the irradiated materials

This content has been downloaded from IOPscience. Please scroll down to see the full text.

2012 J. Phys.: Conf. Ser. 345 012009

(<http://iopscience.iop.org/1742-6596/345/1/012009>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 212.193.78.1

This content was downloaded on 27/03/2015 at 10:48

Please note that [terms and conditions apply](#).

Computer simulation of field ion images of nanoporous structure in the irradiated materials

E.V. Medvedeva¹, S.S. Alexandrova¹, T.A. Belykh²

¹ Institute of Electrophysics, Ural Branch, Russian Academy of Science, Amudsen str., 106, Yekaterinburg, 620016, Russia

² Federal State Autonomous Institution of Higher Professional Education "Ural Federal University named after the first President of Russia B.N. Yeltsin", Mira str. 19, Yekaterinburg, 620002, Russia

E-mail: lena_p@bk.ru; alexandrova.swetlana@gmail.com

Abstract. Computer simulation and interpretation of field ion microscopy images of ion irradiated platinum are discussed. Field ion microscopy technique provides direct precise atomic scale investigation of crystal lattice defects of atomically pure surface of material; at the same time it allows to analyze the structural defects in volume by controlled and sequential removal of surface atoms by electric field. Defects identification includes the following steps: at the first stage the type of crystalline structure and spatial orientation of crystallographic directions were determined. Thus, we obtain the data about exact position of all atoms of the given volume, i.e. the model image of an ideal crystal. At the second stage, the ion image was processed used the program to obtain the data about real arrangement of atoms of the investigated sample. At the third stage the program compares these two data sets, with a split-hair accuracy revealing a site of all defects in a material. Results of the quantitative analysis show that shape of nanopores are spherical or cylindrical, diameter on nanopores was varied from 1 to 5 nm, their depth was found to be from 1 to 9 nm. It was observed that nearly 40% of nanopores are concentrated in the subsurface layer 10 nm thick, the concentration of nanopores decreased linearly with the distance from the irradiated surface.

1. Introduction

It is common knowledge that ion irradiation of metals generates a large number of defects, including vacancies and interstitials, bubbles and dislocation loops [1-3]. The information on the distribution of radiation damages is of great importance for understanding the processes of formation and evolution of defective structure, for an explanation of mechanisms of radiating influence on structure and properties of irradiated material. The aim of this paper is to analyze, using field ion microscopy (FIM), the structure of radiation-induced defects on the atom-free platinum surface and in the platinum subsurface bulk, which were formed by the Ar⁺ ion irradiation. Concerning a possibility of the nanoscale analysis of crystal structure of metals and alloys, the method of field ion microscopy is most informative of existing methods. This method enables one to conduct direct precision study of radiation damages of crystal lattice of a material in the atom scale, to identify large and ultra small pores up to single vacancies and their segregations, to determine their concentration, sizes, shape, and

the distribution over the bulk of irradiated material, to change the specified parameters depending on the radiation fluency.

The obtained data allows us to clarify the mechanism of the effect of radiation on the structure of metal and alloys, which is of great importance for understanding the properties of irradiated materials. As a result, the dynamics and evolution of radiation defects can be related to the macroscopical processes proceeding under the irradiation.

2. Experimental

It is difficult to analyze the modification of the structure and properties of materials subjected to the implantation of ions with average energies of 10–100 keV by using FIM experiments, because the near-surface metal layer with a thickness of tens or hundreds of nanometers (depending on the bombardment regime) is bombarded. Therefore, the samples to be studied were prepared in the form of tip samples with the tip's radius of curvature of 10–30 nm from metal rods by electrochemical polishing. Then, an ion image of Pt in the initial state was obtained. Field emitters certified for ion implantation had atomically smooth tip surfaces close to the spherical one prepared in situ by the field evaporation of surface atoms. If the FIM is used, pure surface of samples is prepared directly in the microscope and is maintained pure during the whole experiment. Irradiation of Pt tip-samples was provided using Ar^+ ions accelerated up to 30 keV with fluencies of $F=10^{18} \text{ cm}^{-2}$ and ion current density of $j=200 \text{ } \mu\text{A/cm}^2$ at $T=573 \text{ K}$. Irradiation was performed in a direction parallel to the axis of the tip-sample. The irradiated tip-samples were inserted again in the field ion microscope and, using photo and video cameras, the field ion micropictures of the surface were recorded during the controlled removal of atomic layers and the experimental results for the subsequent analysis of the defect structure were obtained. The ion images were registered so that the quantity of the evaporated atoms in intervals between pictures was minimum. Such detailed and labor-consuming procedure was necessary for precision revealing of defects of a crystal lattice, which can be overlooked in the case of evaporation of entire atomic plane. The field ion microscope was equipped with a microchannel ion–electron converter increasing the brightness of the surface micropictures by a factor of 10^4 , liquid nitrogen ($T = 77 \text{ K}$), as a rule, served as a cooling agent, and spectrally pure neon was used as an imaging gas. The information on nanopores and their distribution over the subsurface volume of the irradiated material is obtained by means of a computer program complex for interpretation of field ion images.

3. Results and discussion

The radiation damage in Pt was studied after ion bombardment of preliminarily prepared atomically pure and atomically smooth surfaces of field emitters (Fig. 1).

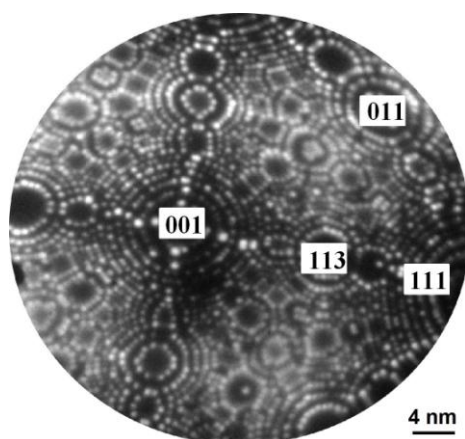


Figure 1. Ion image of the initial atomically pure and atomically smooth platinum surface prior to irradiation.

This is a typical micropicture of the surface of a pure metal with the FCC lattice. The crystal is oriented along the [001], in almost perpendicular direction to the micropicture plane. These contrast points form regular circles (families of planes of the corresponding crystal's region), whose centers are the corresponding poles of the stereographic projection [4]. Figure 2 shows micropicture of surface of irradiated by argon ions Pt. Distortions of the ion contrast and regularities of the pattern of circles were observed in several areas of the surface of the irradiated plate.

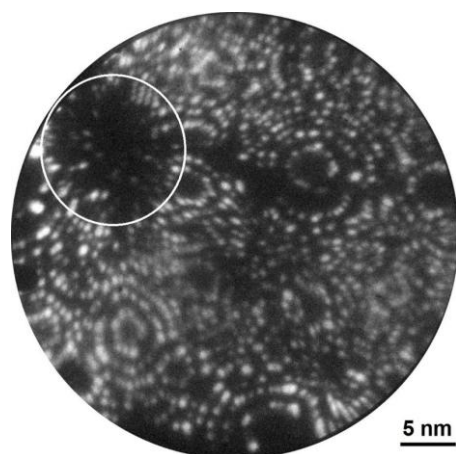


Figure 2. Ion image of pure Pt after irradiation by argon ions (contrast of the nanopore is shown by a circle).

These distortions of the ion contrast in the pattern of circles demonstrate the presence of defects in the crystal structure. Various types of defects induced in materials subjected to some external actions can be identified using contrast available from the literature [5, 6]. In this case, a change in the ion contrast of the irradiated plate compared to the contrast of the initial platinum is due to radiation damage produced by the interaction of ion with the crystal lattice. The structure of defects was analyzed in the material bulk during controlled removal of platinum atoms one by one from the surface by an electric field. The observed radiation damages were the nanopores. Contrast from the nanopores in Pt was registered immediately when the ion image of the surface appeared, and it remained after the surface layers of the irradiated metal were removed (Fig. 2). The ion contrast of nanopores at the moment of the field evaporation of the last atomic layer prior to the formation of a nanopore was registered in the form of craters. Then, as the atomic layers surrounding the defect evaporated, we observed the profile of a defect whose size was a bit less than when the nanopore opened. Finally, the nanopore's exit from the material during the evaporation of atomic layers from the surface ended, as a rule, with a dislocation loop (Fig. 3).

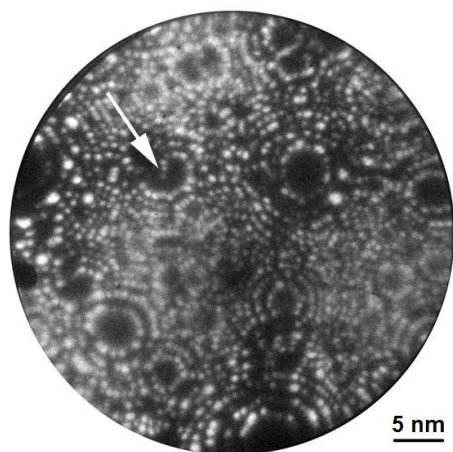


Figure 3. Ion image of Pt after irradiation by ions of Ar^+ (contrast dislocation loop at an exit of a nanopore from the material is shown by an arrow).

It is known that, in the metals, spherical vacancy pores are unstable, they are squeezed in a plane of one of the most dense atom layers of a crystal and form dislocation loops. In the case under consideration, the nanopores represent the bubbles, which are the accumulations of Ar^+ ion gas; they create a pressure upon a cavity wall that compensates a superficial tension and stimulate an increase in a noncompensated flow of vacancies [7].

It should be noted that bulk radiation defects in a layer of 10 nanometers from the irradiated surface have the form of craters. Such surface morphology is a result of erosion. For the given combination of material type of ions, and implantation modes, erosion can proceed by various mechanisms. Firstly, in the course of implantation, the material can be sprayed not as individual atoms, which is typical for beams with the currents of several μA , but in the form of clusters. This is additionally favored by the needle shape of the specimen; a high electric field in the beam plasma is concentrated at the tip of the sample. Secondly, the implantation of inert gases (here, argon) with high fluencies is characterized by the formation of blisters, which will have a shape of craters on the ion image.

For the quantitative analysis of nanoporous structure of the irradiated material, a specially developed computer program complex was used [8]. The principles of defect identification were the following: at the first stage, the type of crystalline structure and spatial orientation of crystallographic directions were determined. Thus, we obtain the data on the exact position of all atoms of the given volume, i.e. the model image of an ideal crystal. At the second stage, the ion image was processed using the program to obtain the data about real arrangement of atoms in sample under investigation. At the third stage, the program compares these two data sets, with a split-hair accuracy revealing the sites of all defects in the material (Fig. 4).

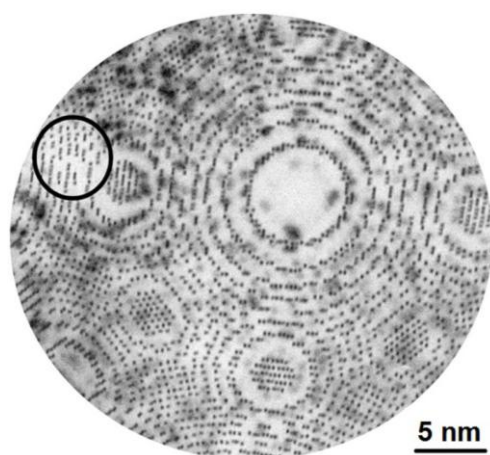


Figure 4. A comparison of the ion image of irradiated Pt with the simulated image of FCC-crystal free of defects (a nanopore is shown by a circle).

The results of the quantitative analysis show that the nanopores were both spherical and cylindrical, the diameter of nanopores varied from 1 to 5 nm, and the depth of nanopores varied from 1 to 9 nm. Successive evaporation by electric field of superficial nuclear layers to depth of 60 nm from the irradiated surface and the application of computer simulation of ion images allowed revealing specific features of formed nanopores. The concentration of nanopores and their distribution over the subsurface volume of the irradiated material were calculated. It was found that nearly 40% of nanopores are concentrated in the subsurface layer 10 nm thick, the concentration of nanopores decreased linearly ($y = -0.084x + 5.154$) with the distance from the irradiated surface (Fig. 5).

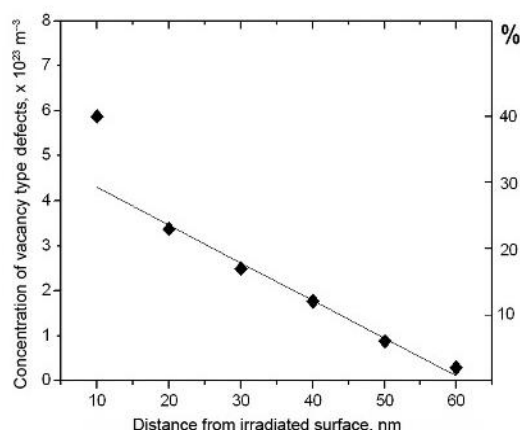


Figure 5. Profile of concentration of defects of vacancy type in Pt irradiated by Ar^+ ions.

These numerical values of coefficients of linear dependence were calculated only for the conditions of above experiment. A deviation of the first experimental point from this dependence can be caused by the fact that, in addition to the mechanism of pore formation, the surface erosion can contribute to the number of volume defects of the vacancy type.

4. Conclusions

Nanoporous structure formed in Pt by ion irradiation was investigated by field ion microscopy. Computer simulation was applied for quantitative analysis of size, shape and concentration of nanopores. It was observed that a decrease in nanopores concentration in the volume with distance from the irradiated surface can be described by linear equation. The analysis of shapes and sizes of nanopores allows us to propose that the nanopores in the samples studied represent gas bubbles formed by argon.

5. Acknowledgments

This work is supported by the Federal Target Program «Scientific and scientific-pedagogical personnel of innovative Russia», State Contract no. P750, May 20, 2010. Also it is supported by the Russian Fund of Basic Researches (the project № 10-02-96003-r_ural_a).

References

- [1] Kirsanov V V, Suvorov A L, Trushin Y V 1985 *The processes of radiation defect formation in metals* (Moscow: Energoatomizdat) p 275
- [2] Beavan L.A, Scanlam R M, Seidman N 1971 The Defect Structure of Depleted zones in Irradiated Tungsten *Acta Metallurgica* **19** 1339
- [3] Gao F, Heinisch H L, Kurtz R J 2009 Migration of vacancies, He interstitials and He-vacancy clusters at grain boundaries in a-Fe *Journal of Nuclear Materials* **386–388** 390–394
- [4] *Field-ion Microscopy* 1968 ed Hred J and Ranganathan S (New York: Plenum Press)
- [5] Muller E W and Tsong T T 1969 *Field-ion Microscopy (Principles and Applications)* (New York: Elsevier)
- [6] Bowkett K M and Smith D A 1970 *Field Ion Microscopy* (Nord-Holland, Amsterdam, London).
- [7] Gribkov V A, Grigoryev F I, Kalin B A, Yakushin V L 2001 *Prospective radiation beam technologies of materials working* ed Kalin B A (Moscow) p 528
- [8] Moore A J W 1962 The structure of atomically smooth spherical surface *J. Phys. Chem. Solids*, **23** 907